Exact Solution of a Two-Species Quantum Dimer Model for Pseudogap Metals

Johannes Feldmeier, Sebastian Huber, and Matthias Punk

Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-University Munich, 80333 Munich, Germany

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We present an exact ground state solution of a quantum dimer model introduced by Punk, Allais, and Sachdev [Quantum dimer model for the pseudogap metal, Proc. Natl. Acad. Sci. U.S.A. 112, 9552 (2015).], which features ordinary bosonic spin-singlet dimers as well as fermionic dimers that can be viewed as bound states of spinons and holons in a hole-doped resonating valence bond liquid. Interestingly, this model captures several essential properties of the metallic pseudogap phase in high-$T_c$ cuprate superconductors. We identify a line in parameter space where the exact ground state wave functions can be constructed at an arbitrary density of fermionic dimers. At this exactly solvable line the ground state has a huge degeneracy, which can be interpreted as a flat band of fermionic excitations. Perturbing around the exactly solvable line, this degeneracy is lifted and the ground state is a fractionalized Fermi liquid with a small pocket Fermi surface in the low doping limit.

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Quantum dimer models have been a very useful tool to study paramagnetic ground states of quantum antiferromagnets. Originally introduced by Rokhsar and Kivelson to elucidate the physics of Anderson’s resonating valence bond (RVB) state in the context of high-temperature superconductors [1–4], these models provide an effective description of low energy singlet excitations in antiferromagnets and feature rich phase diagrams, including a variety of different valence bond solids with broken lattice symmetries, as well as symmetric spin-liquid phases [5–9]. Subsequently, interesting connections to lattice gauge theories and loop gas models have been found, raising interest in quantum dimer models from various perspectives [10–14].

In this work we consider an extension of the Rokhsar-Kivelson (RK) model on the square lattice introduced by Punk, Allais, and Sachdev [1], which provides an effective low-energy description of hole-doped antiferromagnets in two dimensions. The Hilbert space is constructed by hardcore coverings of the square lattice with two flavors of dimers: the standard nearest-neighbor bosonic spin-singlets of the RK model, as well as fermionic dimers carrying charge $+e$ and spin 1/2. These fermionic dimers can be viewed as bound states of a spinon and a holon in hole-doped RVB states [15–21]. It has been argued in Refs. [1,22] that this model features a so-called fractionalized Fermi liquid ground state [23], with a small Fermi surface enclosing an area proportional to the density of doped holes away from half filling. This apparent violation of Luttinger’s theorem, which states that the Fermi surface should enclose an area proportional to the total number of holes with respect to the completely filled band in metallic phases without broken symmetries [24], is possible due to the presence of topological order [25,26].

One of the most interesting aspects of this model is the fact that it captures various properties of the metallic pseudogap phase in underdoped high-$T_c$ cuprate superconductors, such as the presence of a small hole-pocket Fermi surface with a highly anisotropic, electronic quasi-particle residue, providing a potential explanation for the observation of Fermi arcs in photoemission experiments. Moreover, this model exhibits a large pseudogap in the antinodal region of the Brillouin zone around momenta $k \sim (0, \pi)$ and symmetry related points [27].

While previous studies of this quantum dimer model were mostly based on numerical approaches, we present an exact analytical solution for the ground state at an arbitrary density of fermionic dimers in this work. This solution is based on a generalization of the original idea by Rokhsar and Kivelson that the Hamiltonian can be written as a sum of projectors in certain parameter regimes. While it is easy to see that the corresponding ground state is a simple equal weight superposition of all possible dimer coverings in the RK case, this is no longer true in the presence of fermionic dimers, because the equal weight superposition is not antisymmetric under the exchange of two fermions. Nevertheless, it is still possible to construct the exact ground state wave function, as we show in detail below. Interestingly, we find that fermionic excitations are dispersionless and form a flat band at this generalized RK line in parameter space. Perturbing away from the exactly solvable line we can show that the ground state of this model is indeed a fractionalized Fermi liquid at low densities of fermionic dimers.

We start from the dimer model introduced in Ref. [1] and add an additional potential energy term for configurations with pairs of parallel fermionic and bosonic dimers within a
The Hamiltonian $H = H_{\text{RK}} + H_1$ consists of two parts: the standard Rokhsar-Kivelson Hamiltonian for bosonic dimers,

$$H_{\text{RK}} = \sum_{i,j} [-JD_{i,j}^+ D_{i,j}^+ \delta_{i,j} + JD_{i,j}^+ D_{i,j} + V D_{i,j}^+ D_{i,j}^+ D_{i,j}],$$

as well as similar terms with plaquette resonances and potential energy terms between a bosonic and a fermionic dimer

$$H_1 = -t_1 \sum_i [D_{i,x}^+ F_{i,y}^+ F_{i,x}^+ \delta_{i,y} + 3\text{terms}] + v_1 \sum_i [D_{i,x}^+ F_{i,y}^+ F_{i,x,}^+ \delta_{i,y} + 3\text{terms}] - t_2 \sum_i [D_{i,x}^+ F_{i,y}^+ F_{i,x}^+ \delta_{i,y} + 7\text{terms}] - t_3 \sum_i [D_{i,x}^+ F_{i,y}^+ F_{i,x}^+ \delta_{i,y} + 15\text{terms}].$$

Here, $D_{i,j} (F_{i,j})$ is an annihilation operator for a bosonic (fermionic) dimer on the bond emanating from lattice site $i$ in direction $\eta \in \{x, y\}$, while $\bar{\eta} \in \{\bar{x}, \bar{y}\}$ denotes basis vectors in $x$ and $y$ directions (the lattice constant has been set to unity throughout this Letter). Finally, $\bar{\eta}$ denotes the complement of $\eta$, i.e., $\bar{\eta} = x$ if $\eta = y$ and vice versa. The terms which are not explicitly displayed are related by lattice symmetry operations and Hermitian conjugation. Note that in contrast to Ref. [1] we omit a possible spin index for the fermionic dimers. Nevertheless, all our results can be generalized to spinful fermions easily. Further terms involving resonances of two or more fermionic dimers are possible as well, but are not expected to be important in the interesting regime of low doping, where the density of fermionic dimers is small. Moreover, we will focus exclusively on the topological sector of the Hilbert space of hard-core coverings with zero winding number throughout this work [27].

In the next step we identify a line in parameter space which allows us to rewrite the Hamiltonian $H$ as a sum of projectors. As the model then takes a form similar to the original RK Hamiltonian at $J = V$ [4], we shall speak of an RK line in the following. Setting the parameters to $J = V$, $t_0 = 0$ and $v_1 = t_2 = -t_1$, the full Hamiltonian can be expressed graphically as a sum of projectors

$$H = J \sum_{\text{plaq} \neq 0} (\langle 0 | - | 0 \rangle - \langle 0 | - | 0 \rangle) + v_1 \sum_{\text{plaq} \neq 0} P_l$$

where empty (full) ellipses represent bosonic (fermionic) dimers.

As a consequence of the special form of Eq. (3), the Hamiltonian is positive definite, i.e., $\langle \psi | H | \psi \rangle \geq 0$ for all wave functions $\psi$. The ground state can hence be determined by the condition $H | \psi_0 \rangle = E_0 | \psi_0 \rangle = 0$. We now construct ground state wave functions $| \psi_0 \rangle$ in an arbitrary sector of the (conserved) number of fermionic dimers $N_f$. In the following calculation we restrict to the case $N_f = 2$, the generalization to arbitrary fermion numbers is straightforward. We assume the ground state to be a common eigenstate of $H_{\text{RK}}$ and $H_1$. As we already know that the bosonic part $H_{\text{RK}}$ is minimized by an equal weight superposition of all hard-core coverings with bosonic dimers, we define the basis states

$$| (i_1, \eta_1), (i_2, \eta_2) \rangle = \frac{1}{\sqrt{N_f}} F_{i_1, \eta_1}^+ F_{i_2, \eta_2}^+ | 0 \rangle_{(i_1, \eta_1), (i_2, \eta_2)} \otimes \left( \sum_{c \in C_{(i_1, \eta_1), (i_2, \eta_2)}} | c \rangle \right),$$

where the sum runs over all possible bosonic configurations $| c \rangle$ covering the entire lattice with the exception of the bonds $(i_1, \eta_1)$ and $(i_2, \eta_2)$ which are already occupied by fermionic dimers. Note that $H_{\text{RK}} | (i_1, \eta_1), (i_2, \eta_2) \rangle = 0$ is a zero energy eigenstate of $H_{\text{RK}}$ by construction. We choose to normalize $| (i_1, \eta_1), (i_2, \eta_2) \rangle$ with respect to the number $N_f$ of all possible classical dimer configurations on the entire lattice. The norm of such a basis state is hence given by

$$|| (i_1, \eta_1), (i_2, \eta_2) ||^2 = \frac{N_f | (i_1, \eta_1), (i_2, \eta_2) \rangle \langle (i_1, \eta_1), (i_2, \eta_2) |}{N_f} = Q_c | (i_1, \eta_1), (i_2, \eta_2) \rangle,$$

where $Q_c | (i_1, \eta_1), (i_2, \eta_2) \rangle$ is the classical dimer correlation function. $N_{(i_1, \eta_1), (i_2, \eta_2)}$ denotes the number of all classical configurations with two dimers fixed at $(i_1, \eta_1)$ and $(i_2, \eta_2)$. With these correlations we implicitly enforce the hard-core constraint, as any constraint-violating configuration $C$ yields a vanishing norm $Q_c | C \rangle = 0$.

In order to construct a ground state $| \psi_0 \rangle$ of the full Hamiltonian $H = H_{\text{RK}} + H_1$ we start with a general expansion

$$| \psi_0 \rangle = \sum_{i_1, \eta_1, i_2, \eta_2} A_{(i_1, \eta_1), (i_2, \eta_2)} | (i_1, \eta_1), (i_2, \eta_2) \rangle.$$  

Applying the Hamiltonian we obtain

$$H | \psi_0 \rangle = v_1 \sum_{i_1, \eta_1, i_2, \eta_2} \sum_{l} A_{(i_1, \eta_1), (i_2, \eta_2)} P_l | (i_1, \eta_1), (i_2, \eta_2) \rangle.$$
Note that $P_f$ acts nontrivially only on plaquettes containing a single fermionic dimer and thus
\[ P_f(i_1, \eta_1), (i_2, \eta_2) = (\delta_{i_1, i_2} + \delta_{i_1, i_3} + \delta_{i_2, i_3}) P_f(i_1, \eta_1), (i_2, \eta_2). \]  
(9)

Furthermore, we find
\[ \delta_{i_1, i_2} P_f(i_1, \eta_1), (i_2, \eta_2) = \delta_{i_1, i_2} (-1)^{\eta_1} |\phi_f(i_1, \eta_1), (i_2, \eta_2)\rangle \]  
(10)

and similar relations for the remaining three terms of Eq. (9), where we defined the states
\[ |\phi_f(i, \eta)\rangle = \frac{1}{\sqrt{N}} \sum_{\sigma} |\eta\rangle \sigma \phi^{\dagger}_{\langle \sigma \rangle(i, \eta)} |\eta\rangle \]  
(11)

and further $s_{y=x} = 1$, $s_{y=y} = 0$. Again, normalization of these states resorts to classical correlations and effectively projects onto the physical space of hard-core configurations.

Inserting Eq. (10) into Eqs. (9) and (8), and demanding that all coefficients for the states $|\phi_f(i_1, \eta_1), (i_2, \eta_2)\rangle$ vanish results in the two conditions
\[ A_{(i, x), (i, y)} + A_{(i, x), (i, y)} - A_{(i, x), (i, y)} = 0, \]
\[ A_{(i, x), (i, y)} + A_{(i, x), (i, y)} - A_{(i, x), (i, y)} = 0, \]  
(12)

which can be solved by a simple product ansatz
\[ A_{(i, x), (i, y)} = a_{i, x} a_{i, y}, \]
leading to
\[ a_{i, x} a_{i, y} + a_{i, x} a_{i, y} - a_{i, x} a_{i, y} = 0 \]  
(13)

for $m = 1, 2$. At this point, the generalization to an arbitrary number of fermionic dimers in the system is straightforward and can be done by extending Eq. (13) to $m = 1, \ldots, N_f$. We introduce the lattice momenta $p_m$ and make the ansatz
\[ a_{i, x} a_{i, y} = a_{i, x} a_{i, y}(p_m) = C_{p_m}(p_m) e^{ip_m i_m}, \]  
(14)

where the factors $C_{p_m}(p)$ can be interpreted as weight factors for the two possible dimer orientations and $i_m$ denotes the lattice position of site $i_m$. Using this ansatz in Eq. (13) and choosing the normalization $|C_{p}(p)|^2 + |C_{p}(p)|^2 = 4/N$ for later convenience, we obtain
\[ C_{p}(p) = \frac{2}{\sqrt{N}} \frac{1 + e^{ip_m}}{\sqrt{1 + e^{ip_m}}^2 + 1 + e^{ip_m}}, \]  
(15)

where $N$ is the number of lattice sites. One can thus write exact ground states of $H$ on the RK line with two fermionic dimers as
\[ |\psi(0)\rangle = |p_1, p_2\rangle = \sum_{i_1, \eta_1, i_2, \eta_2} a_{i_1, \eta_1}(p_1) a_{i_2, \eta_2}(p_2) |i_1, \eta_1\rangle, (i_2, \eta_2)\rangle. \]
(16)

Note that $p_1$ and $p_2$ take arbitrary values in the first Brillouin zone and $|p_1, p_2\rangle = -|p_2, p_1\rangle$ is antisymmetric under the exchange of $p_1$ and $p_2$. The ground state degeneracy corresponds to the $N(N - 1)/2$ possibilities to choose $p_1, p_2$. This result implies that fermionic dimers have a flat dispersion at the RK line, which we confirmed independently by an exact diagonalization of the Hamiltonian on the RK line for a finite system. We also note that the state in Eq. (16) is properly normalized in the limit $N \to \infty$.

For an arbitrary number $N_f$ of fermionic dimers the ground states take the form $|\psi(0)\rangle = |p_1, \ldots, p_{N_f}\rangle$ and there are $N!((N - N_f)!N_f!)$ possibilities to choose the $N_f$ momenta $(p_1, \ldots, p_{N_f})$. It is important to emphasize that the states $|p_1, \ldots, p_{N_f}\rangle$ are in general not linearly independent, and the number of possible momenta $(p_1, \ldots, p_{N_f})$ does not correspond to the ground state degeneracy in sectors with a large density of fermionic dimers. In fact, it is easy to see that the number of possible choices for the $N_f$ momenta exceeds the number of basis states at large $N_f$. However, in the low doping limit
\[ N_f = \text{const}, \quad N \to \infty, \quad (17) \]
the $|p_1, \ldots, p_{N_f}\rangle$ become orthonormal and we indeed obtain the ground state degeneracy via the above relation.

It is instructive to note how the states $|p\rangle$ for $N_f = 1$ are related to the usual bosonic RK ground state, if the fermionic dimer is replaced with a bosonic one. As shown in the Supplemental Material [28], the purely bosonic states $|p\rangle$ vanish identically for $p \neq 0$, which only leaves the ordinary RK state with $p = 0$, i.e., the equal superposition of all bosonic dimer coverings, as the unique ground state.

In the following we want to study how perturbations $\Delta H$ of the Hamiltonian away from the RK line change the ground state structure. We consider perturbations of the form $H + \Delta H = H(i_t + \delta i_t)$. As expected, the huge ground-state degeneracy will be lifted and the fermions will acquire a dispersion. The perturbative ground state in the vicinity of the RK line is then unique and similar to a Fermi gas, where the lowest energy momentum states $p_m$ will be filled with $N_f$ fermions. We restrict our discussion to the limit of Eq. (17), where the degenerate ground states $|p_1, \ldots, p_{N_f}\rangle$ are properly normalized. Moreover, we only
consider terms in $\Delta H$ which exchange two dimers, i.e., $\delta t_1$ and $\delta t_3$ terms. Flip interactions like $t_2$ will be neglected for simplicity, but can be included as well.

Within first order perturbation theory the eigenstates remain unchanged, but their energy is given by $\Delta E = \langle p_1, \ldots, p_{N_f} | \Delta H | p_1, \ldots, p_{N_f} \rangle$. Evaluating the matrix elements for the case $N_f = 2$ we get $\Delta E = \epsilon(p_1) + \epsilon(p_2)$ with

$$
\epsilon(p) = -4 \sum_{j=1}^{3} \delta t_j Q_c[(0, x), (r_j, x + \eta_j)]
\times \sum_{\eta} \left[ 1 + e^{ip_\eta} \right] \left[ 1 + e^{-ip_\eta} \right]^{S_\eta} e^{-ip_\eta} \sum_{s=1}^{S_\eta} e^{-t_s p_\eta},
$$

where $r_j$ and $\eta_j$ correspond to displacement vector and relative change in orientation for a given $t_j$ process which annihilates a fermionic dimer with initial orientation $\eta$. The sum over the possible $r_j$ corresponding to a given $t_j$ depends on the orientation index $\eta$ and runs from $s = 1$ to $S_\eta = 2$, $S_\eta = 8$. The classical probabilities $Q_c[(0, x), (r_j, x + \eta_j)]$ are $1/8$ and $1/(4\pi)$ for $t_1$ and $t_3$, respectively, and can be obtained from the exact solution of the classical dimer problem [29,30]. Details of the computation can be found in the Supplemental Material [28]. We show an example for $\epsilon(p)$ together with exact diagonalization results on a $6 \times 6$ lattice with one fermionic dimer and twisted boundary conditions in Fig. 1. For $|\delta t_j| \ll |v_1|$, $J$ we find excellent agreement. Note the formation of hole pockets around $(\pi/2, \pi/2)$ at a finite density of fermionic dimers for perturbations in $\delta t_3$.

The preceding results demonstrate that the energy of a state $|p_1, \ldots, p_{N_f}\rangle$ is additive in the single particle energies in the low doping limit, indicating a system with Fermi-liquid like behavior. Now we show that in the same limit the ground states $|p_1, \ldots, p_{N_f}\rangle$ can be constructed using creation and annihilation operators that fulfill canonical fermionic anticommutation relations.

We start by defining the vacuum state of the theory to be the usual RK ground state, i.e., $|0'\rangle = |\text{RK}\rangle$, which corresponds to the equal weight superposition of all possible hard-core coverings of the lattice with bosonic dimers. We add the star in this notation to emphasize the difference to the vacuum state $|0\rangle$ used previously. By defining the operator

$$
f_\eta = \sum_{i} a_{i,\eta} (p) F_{i,\eta}^\dagger D_{i,\eta},
$$

we can express the possible ground states along the RK line as

$$
|p_1, \ldots, p_{N_f}\rangle = \prod_{i=1}^{N_f} f_\eta |0\rangle.
$$

We aim to show that the corresponding Hamiltonian $H = \sum_p \epsilon(p) f_\eta^\dagger f_\eta$ describes the model in the vicinity of the RK line as a system of noninteracting fermionic excitations. We hence need to show that the canonical anticommutation relations

$$
\{f_\eta^\dagger, f_\eta\} = \delta_{p_\eta},
$$

are satisfied in the limit of Eq. (17). Note that we require specification of the Hilbert space on which Eq. (21) is supposed to hold. In usual fermionic theories the anticommutation relations must hold on the Fock space spanned by the set of states $\{\prod_{i=1}^{N_f} c_{i,\eta}^\dagger |0\rangle\}$. In direct analogy we demand that in our model Eq. (21) should hold on the Hilbert space spanned by the states $\{\prod_{i=1}^{N_f} f_\eta |0\rangle\}$. Thus, even though the operators of Eq. (19) do not constitute fermionic operators on a Hilbert space built upon the actual vacuum state $|0\rangle$, we still can prove them to be fermionic within our relevant Hilbert space. The quantity we aim to compute is now $\{f_\eta^\dagger, f_\eta\} |0\rangle$ and we want to show that this expression yields $\delta_{p_\eta} |0\rangle$. From the relation $\{f_\eta^\dagger, f_\eta\} = \sum_{i,\eta} a_{i,\eta}^\dagger (p_\eta) N_{i,\eta}$, where $N_{i,\eta}$ corresponds to the total dimer number operator on the link $(i, \eta)$, we deduce

FIG. 1. Comparison between $\epsilon(p)$ from Eq. (18) (left) and the dispersion obtained from exact diagonalization (ED) for $6 \times 6$ lattice sites with one fermionic dimer and twisted boundary conditions (middle) for $J = V = 1$, $v_1 = t_2 = -t_1 = 1$ and $\delta t_3 = -0.02$. Right: corresponding line cut through the Brillouin zone [blue line with dots: ED, orange line: Eq. (18)].
that \(|\{f^+_p, f^-_p\}|0^+\rangle|^2 \) is given by the Fourier transformed classical dimer correlation function (see the Supplemental Material for details [28]), which reduces to \(\delta_{p_1,p_2} \) for \(N \to \infty \) as claimed, with corrections of order \(O[\log(N)/N] \). The appearance of the total dimer number operator \(\hat{N}_{i,j} \) then ensures that this result remains valid for all states in our Hilbert space provided that Eq. (17) be fulfilled. Beyond this limit, where the Fourier transform of the classical dimer correlation function reduces to a delta function, we show in the Supplemental Material that \(\rho_{\text{RK}} \) is given by the Fourier transformed Fermi liquid ground state is stable over a wider parameter regime. Indeed, the \(U(1) \) spin liquid in the square lattice RK model at half filling is unstable towards confining, symmetry broken states away from the special RK point \(J = V \). On nonbipartite lattices an extended \(Z_2 \) spin liquid phase exists, however [7]. Analogous considerations hold for hole doped RK models [34,35] as well as the fractionalized Fermi liquid phase discussed here [26,36]. Including diagonal, next-nearest neighbor dimers in our model is an interesting point for future study. In conclusion, our results provide a rare example of a strongly correlated, fermionic lattice model in two dimensions, which is exactly solvable and potentially relevant for the description of the metallic pseudogap phase in underdoped cuprates.

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